Li conduction in Li2S-P2S5 glasses: insights from dynamics and polarizability

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Abstract

We investigated the dynamical and polarizable properties of Li2S-P2S5 glasses, which is a fast Li-conducting material, by performing ab initio molecular dynamics simulations for 300 ps at 300 K. Structural properties a zone analysis based on Li migration highlighted the effective path along which Li diffuses in the materials. Our resultssuggested that all the Li ions did not have constant mobility, indicating that some of the Li ions were effectively available for conduction. The origin of the path that would support effective Li diffusion was analyzed in terms of the dynamics and polarizability of the sulfur surrounding the Li migration path.

Keywords: solid state electrolytes, ab initio molecular dynamics, polarizability

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